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SOME NOVEL FEATURES OF THE BANDS IN HTSC

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Abstract—We have calculated the energy dispersions, spectral weights and density of states for two relevant bands near the Fermi level in layered cuprates. Calculated energy dispersion and density of states seem to be consistent with the photoemission data.

Keywords: Layered cuprates, strong correlations, energy dispersion.

The photoemission data give the evidence for an unusual narrow band near the Fermi level in doped cuprates. We refer this band to an oxygen hole motion on a background of copper sites, the oxygen hole spin having a strong singlet coupling to the copper spin. The calculations of energy dispersion showed [1,2] that this band is indeed narrow and well consistent with the photoemission data [3] within the experimental accuracy. Here we report new variant calculations of the energy dispersion, when the singlet copper–oxygen state is assumed to be a combination of Zhang–Rice singlet, Cu^{3+} ($S = 0$) and neutral oxygen.

We start from the ordinary Hamiltonian, including Coulomb repulsion and hopping terms. The basis of wave functions is as follows:

$$|\sigma_d> = d_\sigma^+|0>,\ |\sigma_p> = p_\sigma^+|0>\ \ |dd> = d_\uparrow^+ d_\downarrow^+|0>,$$
$$|pp> = p_\uparrow^+ p_\downarrow^+|0>,\ \ |pd> = \frac{1}{\sqrt{2}}(p_\uparrow^+ d_\downarrow^+ - p_\downarrow^+ d_\uparrow^+)|0>,$$

where $|0>$ is vacuum, which corresponds to $Cu^+(d^{10})$ state, d^+ is a creation operator for copper hole in $|x^2 - y^2>$ state and p_σ is a Wannier-like operator for oxygen hole [4].

In order to calculate the quasiparticle spectrum we perform three successive transformations. After the first Hubbard-like transformation, we do the second canonical transformation of the type

$$\psi^{\sigma_d,0} = c_d X^{\sigma_d,0} + c_p X^{\sigma_p,0},$$
$$\psi^{pd,0} = c_{dd} X^{dd,0} + c_{pd} X^{pd,0} + c_{pp} X^{pp,0}.$$

As a result of such two trannsformations, the one-site Hamiltonian is diagonalized and can be written as:

$$H_0 = E_d \sum \psi^{\sigma_d,\sigma_d} + E_p \sum \psi^{\sigma_p,\sigma_p} + E_{dd}\psi^{dd,dd} + E_{pd}\psi^{pd,pd} + E_{pp}\psi^{pp,pp}.$$

Here

$$E_{d,p} = \frac{\epsilon_d + \epsilon_p}{2} \pm \frac{1}{2}[(\epsilon_p - \epsilon_d)^2 + 4t_0^2]^{\frac{1}{2}},$$

and E_{dd} , E_{pp} and E_{pd} are determined by equation

$$\begin{vmatrix} I_{dd} + 2\epsilon_d - E & 0 & \sqrt{2}t_0 \\ 0 & I_{pp} + 2\epsilon_p - E & \sqrt{2}t_0 \\ \sqrt{2}t_0 & \sqrt{2}t_0 & I_{pd} + \epsilon_p + \epsilon_d - E \end{vmatrix} = 0.$$

ϵ_d and ϵ_p are the energies of copper and oxygen holes, I_{dd}, I_{pp}, I_{pd} are Coulomb repulsion parameters, $t_0 = -2\lambda_0 t_{pd}$ is hybridization parameter.

It is clear that the low quasiparticle excitation energies are $E_{pd} - E_p$, E_d and $E_{pd} - E_d$. For an isolator, the band E_d is fully occupied,so it is natural to call it as the lower "copper Hubbard" band. The band $E_{pd} - E_d$ corresponds to the singlet correlated oxygen band [1,2]. Both bands have unusual features. Let us write down the equation for the chemical potential. The completeness condition is fulfilled in following form:

$$\psi^{0,0} + \psi^{\uparrow,\uparrow} + \psi^{\downarrow,\downarrow} + \psi^{pd,pd} = 1,$$

and anticommutator relations are:

$$[\psi^{pd,\bar{\sigma}_p}, \psi^{\bar{\sigma}_p,pd}]_+ =< \psi^{pd,pd} >,$$
$$[\psi^{pd,\bar{\sigma}_d}, \psi^{\bar{\sigma}_d,pd}]_+ = \frac{1}{2} + \frac{\delta}{2} = P_{pd},$$
$$[\psi^{\sigma_d,0}, \psi^{0,\sigma_d}]_+ = \frac{1}{2} - \frac{\delta}{2} = P_d.$$

First of all we see that at the number of extra hole per site $\delta = 0$ we get exactly Hubbard-like isolator. So the problem disappears which took place in early of charge transfer isolator theory. On the basis of relations one can find the spectral weight (number of occupied states over number of allowed states) of singlet correlated band as $f_p = 2\delta/(1 + \delta)$. For so called electron-doped layered cuprates the carriers reside at E_d band only. Using then $\delta = -\delta_e$ one has $f_d = (1 - \delta_e)/(1 + \delta_e)$.

The energy dispersion of the bands $\epsilon_d^* = E_d$ and $\epsilon_p^* = E_{pd} - E_d$ are described by the hopping Hamiltonian:

$$H_{hop} = \sum t_{ij}^{(1)} \psi^{pd,\bar{\sigma}_d} \psi^{\bar{\sigma}_d,pd} + \sum t_{ij}^{(2)} \psi_i^{\sigma_d,0} \psi_j^{0,\sigma_d} +$$